

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: Christina Johnson Examiner #: 77266 Date: 9-13-04
Art Unit: 1725 Phone Number: 272-1176 Serial Number: 10/617,852
Mail Box and Bldg/Room Location: 6C61 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: _____

Inventors (please provide full names): _____

Earliest Priority Filing Date: _____

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

Please see attached.

(NOT MUCH OUT THERE THAT WAS CLOSE.)

STAFF USE ONLY

Searcher: Ed

Searcher Phone #: _____

Searcher Location: _____

Date Searcher Picked Up: _____

Date Completed: 9-17-04

Searcher Prep & Review Time: _____

Clerical Prep Time: _____

Online Time: _____

Type of Search

NA Sequence (#) _____

AA Sequence (#) _____

Structure (#) _____

Bibliographic _____

Litigation _____

Fulltext _____

Patent Family _____

Other _____

Vendors and cost where applicable

STN _____

Dialog _____

Questel/Orbit _____

Dr.Link _____

Lexis/Nexis _____

Sequence Systems _____

WWW/Internet _____

Other (specify) _____

CLAIMS:

1. A process for preparing a crystalline silicoaluminophosphate molecular sieve, which process comprises; forming a reaction mixture comprising a source of alumina, a source of phosphate, a source of silica and at least one organic template which comprises one or more tertiary dialkylbutylamines, wherein the alkyl groups are not butyl, inducing crystallization of crystalline molecular sieve, and recovering the crystalline molecular sieve.
2. A process as claimed in claim 1, further comprising the step of calcining the crystalline molecular sieve.
3. A process as claimed in claim 1, wherein the one or more tertiary dialkylbutylamines have the general formula (I):
$$(R)(R')N-(C_4H_9) \quad (I)$$
wherein R and R', which may be the same or different groups, are substituted or un-substituted aliphatic or cycloaliphatic groups, except butyl groups.
4. A process as claimed in claim 3, wherein R and R' are linear alkyl groups, but not butyl groups.
5. A process as claimed in claim 3, wherein R and R' are cycloaliphatic groups.
6. A process as claimed in claim 3, wherein R and R' are linear or branched alcohol groups, or linear or branched amine-containing groups.
7. A process as claimed in claim 3, wherein R and R' contain an alkyl group having from 1 to 3 or 5 to 12 carbon atoms.

8. A process as claimed in claim 3, wherein R and R' contain an alkyl group having from 1 to 3 or 5 or 6 carbon atoms.
9. A process as claimed in claim 3, wherein R and R' contain an alkyl group having from 1 to 3 or 5 carbon atoms.
10. A process as claimed in claim 3, wherein R and R' contain an alkyl group having from 1 to 3 carbon atoms.
11. A process as claimed in claim 3, wherein R and R' are independently one of the following alkyl moieties: methyl, ethyl, n-propyl, iso-propyl, n-pentyl, iso-pentyl, n-hexyl, iso-hexyl, heptyl, iso-heptyl, n-octyl, iso-octyl, n-decyl, iso-decyl, n-undecyl, iso-undecyl, n-dodecyl and iso-dodecyl.
12. A process as claimed in claim 11, wherein R and R' are independently methyl, ethyl and propyl, most preferably methyl.
13. A process as claimed in claim 3, wherein the $-C_4H_9$ group in formula (I) is n-butyl.
14. A process according to claim 1, wherein the process is for the manufacture of a silicoaluminophosphate molecular sieve of framework type AEL.
15. The process of claim 14, wherein the molar ratio of organic template to Al_2O_3 in the synthesis mixture is less than 3.
16. A process according to claim 1, wherein the process is for the manufacture of a silicoaluminophosphate molecular sieve of framework type CHA.

17. The process of claim 16, wherein the molar ratio of organic template to Al_2O_3 in the synthesis mixture is 2 or greater.
18. The process of claim 16, wherein the molar ratio of organic template to Al_2O_3 in the synthesis mixture is 3 or greater.
19. A process according to claim 1, wherein the process is for the manufacture of a silicoaluminophosphate molecular sieve of framework type CHA or AEL and wherein the molar ratio of $\text{P}_2\text{O}_5/\text{Al}_2\text{O}_3$ ratio in the synthesis mixture is within the range 0.8 to 1.3.
20. A silicoaluminophosphate molecular sieve, substantially of CHA framework type, comprising within its intra-crystalline structure at least one template which contains one or more tertiary dialkylbutylamines, wherein the alkyl groups are not butyl.
21. The silicoaluminophosphate molecular sieve of claim 20, wherein the one or more tertiary dialkylbutylamines is N,N-dimethylbutylamine.
22. The silicoaluminophosphate molecular sieve of claim 21, wherein the molecular sieve is SAPO-34.
23. A silicoaluminophosphate molecular sieve, substantially of AEL framework type, comprising within its intra-crystalline structure at least one template which contains one or more tertiary dialkylbutylamines, wherein the alkyl groups are not butyl.
24. The silicoaluminophosphate molecular sieve of claim 23, wherein the one or more tertiary dialkylbutylamines is N,N-dimethylbutylamine.

25. The silicoaluminophosphate molecular sieve of claim 24, wherein the molecular sieve is SAPO-11.
26. The silicoaluminophosphate molecular sieve of claim 23, having a platelet morphology.
27. A method for the manufacture of a formulated catalyst composition, which method comprises forming a mixture comprising at least one silicoaluminophosphate molecular sieve according to claim 20 with at least one formulating agent, to form a catalyst composition.
28. A method for the manufacture of a formulated catalyst composition, which method comprises forming a mixture comprising at least one silicoaluminophosphate molecular sieve according to claim 23 with at least one formulating agent, to form a catalyst composition.
29. A formulated molecular sieve composition comprising at least one silicoaluminophosphate molecular sieve according to claim 20 in admixture with at least one formulating agent.
30. A formulated molecular sieve composition comprising at least one silicoaluminophosphate molecular sieve according to claim 23 in admixture with at least one formulating agent.

SYNTHESIS OF SILICOALUMINOPHOSPHATESABSTRACT

The invention is directed to a method of synthesising silicoaluminophosphate molecular sieves and in particular those of framework type CHA and AEL. The method uses synthesis templates that comprise one or more tertiary dialkylbutylamines, wherein the alkyl groups are not butyl. The use of such templates, especially N,N-dimethylbutylamine, results in SAPO-11 of a desirable platelet morphology.

* * * * *

=> file reg

FILE 'REGISTRY' ENTERED AT 19:00:14 ON 17 SEP 2004
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=> display history full 11-

FILE 'LREGISTRY' ENTERED AT 16:18:16 ON 17 SEP 2004
L1 STR

FILE 'REGISTRY' ENTERED AT 16:24:36 ON 17 SEP 2004
L2 SCR 1840 OR 1874 OR 1312 OR 1267 OR 1929 OR 1918 OR 2043
L3 SCR 1609
L4 50 SEA SSS SAM L1 AND L3 NOT L2
L5 202482 SEA SSS FUL L1 AND L3 NOT L2
SAV TEM L5 JOH852/A

FILE 'LREGISTRY' ENTERED AT 16:27:55 ON 17 SEP 2004
L6 STR
L7 STR

FILE 'REGISTRY' ENTERED AT 16:39:26 ON 17 SEP 2004
L8 50 SEA SUB=L5 SSS SAM L6 NOT L7
L10 6 SEA SUB=L5 SSS SAM L6 NOT (L7 OR L9)
L11 581 SEA SUB=L5 SSS FUL L6 NOT (L7 OR L9)
SAV L11 JOH852A/A

FILE 'LREGISTRY' ENTERED AT 16:52:24 ON 17 SEP 2004
L12 STR

FILE 'REGISTRY' ENTERED AT 16:58:44 ON 17 SEP 2004
L13 15 SEA SUB=L5 SSS SAM L12
L14 SCR 1839
L15 10 SEA SUB=L5 SSS SAM L12 NOT L14
L16 4 SEA SUB=L5 SSS SAM (L12 NOT L9) NOT L14
L17 1100 SEA SUB=L5 SSS FUL (L12 NOT L9) NOT L14
SAV L17 JOH204/A

FILE 'HCA' ENTERED AT 17:48:22 ON 17 SEP 2004
L18 28538 SEA SAPO OR S(W)A(W)P(W)O OR CHA OR C(W)H(W)A OR AEL OR
A(W)E(W)L OR (MOL# OR MOLECULAR?) (2A) (SIEVE# OR SIEVING#
OR SIEVEING#) OR ?SILICOALUMINOPHOSPHAT? OR ?ALUMINOSILIC
OPHOSPHAT? OR (SILICO OR SILICON OR SI) (3A) (ALUMINO OR
ALUMINUM# OR AL) (3A) (PHOSPHATE# OR PO4)
L19 4500 SEA SAPO OR S(W)A(W)P(W)O OR CHA OR C(W)H(W)A OR AEL OR

A(W)E(W)L OR ?SILICOALUMINOPHOSPHAT? OR ?ALUMINOSILICOPHOSPHAT? OR (SILICO OR SILICON OR SI) (3A) (ALUMINO OR ALUMINUM# OR AL) (3A) (PHOSPHATE# OR PO4)
 L20 336 SEA ?ALUMINOPHOSPHOSILICAT? OR ?PHOSPHOALUMINOSILICAT?
 OR ?PHOSPHSILICOALUMINAT? OR ?SILICOPHOSPHOALUMINAT?
 L21 108386 SEA (ZEOLIT? OR ANALCIME# OR WAIRAKITE# OR POLLUCITE# OR SODALITE# OR ZK5 OR ZSM5 OR (ZK OR ZSM) (W)5 OR LINDE#(W)A OR FAUJASITE# OR CHABAZITE# OR GMELINITE# OR ERIONITE# OR OFFRETTITE# OR LEVYNITE# OR NATROLITE# OR SCOLOCITE# OR MESOLITE#)/BI,AB
 L22 11911 SEA (EDINGTONITE# OR THOMSONITE# OR GONNARDITE# OR PHILLIPSITE# OR STILBITE# OR HARMOTOME# OR GISMONDINE# OR GARRONITE# OR MORDENITE# OR DACHIARDITE# OR ACHIARDITE# OR HEULANDITE# OR BREWSTERITE# OR EPISTILBITE# OR YUGAWARALITE# OR LAUMONTITE#)/BI,AB
 L23 1163 SEA (FERRIERITE# OR PAULINGITE#)/BI,AB
 L24 48792 SEA TEMPLAT?
 L25 1437 SEA L11
 L26 2513 SEA L17
 L27 0 SEA L25 AND (L19 OR L20)
 L28 0 SEA L25 AND L18
 L29 4 SEA L25 AND (L21 OR L22 OR L23)
 L30 0 SEA L29 AND L24
 L31 3 SEA L25 AND L24

FILE 'REGISTRY' ENTERED AT 17:56:37 ON 17 SEP 2004
 E N,N-DIMETHYLBUTYLAMINE/CN

L32 1 SEA "N,N-DIMETHYLBUTYLAMINE"/CN

FILE 'HCA' ENTERED AT 17:57:45 ON 17 SEP 2004

L33 355 SEA L32
 L34 3 SEA L33 AND ((L18 OR L19 OR L20 OR L21 OR L22 OR L23))
 L35 107631 SEA PLATELET?
 L36 449385 SEA MORPH?
 L37 5 SEA L25 AND L35
 L38 121 SEA L25 AND L36
 L39 3 SEA L37 AND L38
 L40 12 SEA L29 OR L31 OR L34 OR L37 OR L39

FILE 'HCAPLUS' ENTERED AT 18:01:13 ON 17 SEP 2004

L41 25608 SEA CAO ?/AU
 L42 14478 SEA SHAH ?/AU
 L43 1967 SEA BRODY ?/AU
 L44 0 SEA L41 AND L42 AND L43
 L45 23 SEA L41 AND L42
 L46 355 SEA L32
 L47 0 SEA L45 AND L46
 L48 1555 SEA CAO G?/AU

L49 898 SEA SHAH M?/AU
L50 9 SEA L48 AND L49
D L50 1-9 TI
SEL L50 1-5 RN

FILE 'REGISTRY' ENTERED AT 18:04:53 ON 17 SEP 2004
L51 63 SEA (108-00-9/BI OR 108-01-0/BI OR 1938-58-5/BI OR
L52 17 SEA L51 AND L5

FILE 'HCA' ENTERED AT 18:07:43 ON 17 SEP 2004
L53 9 SEA L48 AND L49
L54 0 SEA L40 AND L53

FILE 'REGISTRY' ENTERED AT 18:08:51 ON 17 SEP 2004
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L56 1 SEA L32 AND L11
L57 0 SEA L32 AND L51
L58 0 SEA L17 AND L52

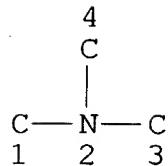
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L59 10 SEA L26 AND ((L18 OR L19 OR L20 OR L21 OR L22 OR L23))
L60 5 SEA L26 AND L24
L61 20 SEA L26 AND L35
L62 317 SEA L26 AND L36
L63 12 SEA L61 AND L62

FILE 'REGISTRY' ENTERED AT 18:23:06 ON 17 SEP 2004
E DIMETHYLCYCLOHEXYLAMINE/CN
L64 1 SEA "DIMETHYLCYCLOHEXYLAMINE HYDROCHLORIDE"/CN
D FIDE
L65 1 SEA 98-94-2
L66 1 SEA L65 AND L17

FILE 'HCA' ENTERED AT 18:25:12 ON 17 SEP 2004
L67 794 SEA L66
L68 3 SEA L67 AND ((L18 OR L19 OR L20 OR L21 OR L22 OR L23))
L69 4 SEA L67 AND L24
L70 1 SEA L67 AND L35
L71 53 SEA L67 AND L36
L72 6 SEA L68 OR L69 OR L70
L73 26 SEA L59 OR L60 OR L63 OR L72

FILE 'REGISTRY' ENTERED AT 19:00:14 ON 17 SEP 2004

=> d 111 que stat
L1 STR



NODE ATTRIBUTES:

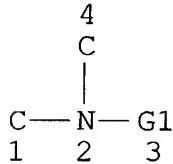
NSPEC IS RC AT 1
 NSPEC IS RC AT 4
 CONNECT IS E3 RC AT 2
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 4

STEREO ATTRIBUTES: NONE

L2 SCR 1840 OR 1874 OR 1312 OR 1267 OR 1929 OR 1918 OR 2043 O
 R 1611
 L3 SCR 1609
 L5 202482 SEA FILE=REGISTRY SSS FUL L1 AND L3 NOT L2
 L6 STR



VAR G1=N-BU/I-BU/S-BU/T-BU

NODE ATTRIBUTES:

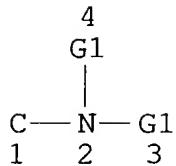
NSPEC IS RC AT 1
 NSPEC IS RC AT 4
 CONNECT IS E3 RC AT 2
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 4

STEREO ATTRIBUTES: NONE

L7 STR



VAR G1=N-BU/S-BU/I-BU/T-BU

NODE ATTRIBUTES:

NSPEC IS RC AT 1
 CONNECT IS E3 RC AT 2
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 4

STEREO ATTRIBUTES: NONE

L9 STR

~~A—X—A~~ ~~A—X—A~~ G1 9
 @1 2 @5 6

VAR G1=1/5

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 5

STEREO ATTRIBUTES: NONE

L11 581 SEA FILE=REGISTRY SUB=L5 SSS FUL L6 NOT (L7 OR L9)

100.0% PROCESSED 59954 ITERATIONS
 SEARCH TIME: 00.00.01

581 ANSWERS

=> file hca

FILE 'HCA' ENTERED AT 19:00:53 ON 17 SEP 2004

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=> d 140 1-12 cbib abs hitstr hitind

L40 ANSWER 1 OF 12 HCA COPYRIGHT 2004 ACS on STN
141:185928 Nucleic acid sequencing using nicking agents and linear or exponential amplification under isothermal conditions. Van Ness, Jeffrey; Galas, David J.; Van Ness, Lori K. (Keck Graduate Institute, USA). PCT Int. Appl. WO 2004067764 A2 20040812, 145 pp. DESIGNATED STATES: W: AE, AE, AG, AL, AL, AM, AM, AM, AT, AT, AU, AZ, AZ, BA, BB, BG, BG, BR, BR, BW, BY, BY, BZ, BZ, CA, CH, CN, CN, CO, CO, CR, CR, CU, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EC, EE, EE, EG, ES, ES, FI, FI, GB, GD, GE, GE, GH, GM, HR, HR, HU, HU, ID, IL, IN, IS, JP, JP, KE, KE, KG, KG, KP, KP, KP, KR, KR, KZ, KZ, KZ, LC, LK, LR, LS, LS, LT, LU, LV, MA, MD, MD, MG, MK, MN, MW, MX, MX, MZ, MZ, NA, NI. (English). CODEN: PIXXD2. APPLICATION: WO 2004-US2719 20040129. PRIORITY: US 2003-PV443597 20030129.

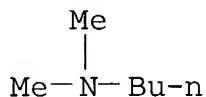
AB A new class of isothermal reactions for sequencing short stretches of DNA is provided that overcomes the disadvantages of traditional sequencing that employ tags or labels. This class includes a linear amplification method and several versions of an exponential amplification scheme. The reactions are simple, flexible, and require no special cycling of conditions. The reactions depend entirely for their rate of amplification on the mol. parameters governing the interactions of the mols. in the reaction. Because of the balance between the thermal properties of the DNA oligonucleotides and the enzymes used, the optimum temp. of the reaction with these enzymes is about 60°. The exponential version of the method, designated the exponential amplification reaction (EXPAR), is an isothermal, mol. chain reaction in that the products of one reaction catalyze further reactions of that copy and sequence triggering oligonucleotides. The linear version of the method is the basic sequencing reaction upon which EXPAR is based. By generating an amplification-template, a linear amplification of ladders of oligonucleotides are generated by coupling a nicking enzyme (e.g., N.BstNbI) and a polymerase in the isothermal reaction. The ladder of oligonucleotides from the linear amplification differ as a single base which can usefully be sep'd. by sequence or length using liq. chromatog., which can be coupled to electrospray ionization time-of-flight (ESI-TOF) mass spectrometry. Foreknowledge of the sequence of the individual or organism is not necessary as it is possible to generate the fragments de novo from genomic DNA. The methods described permit the creation of an assay panel of diagnostic sequences that can identify any organism or individual. In some cases, the ladder of oligonucleotides from the linear sequencing reaction can then be coupled to an isothermal method for exponentially amplifying the triggering sequences in true chain reactions. The triggering and amplification reaction can be made a homogeneous assay in which 108-109-fold amplification can be

achieved in as little as 3 min.

IT 927-62-8, N,N-Dimethylbutylamine
 (sequencing kit contg.; nucleic acid sequencing using nicking
 agents and linear or exponential amplification under isothermal
 conditions)

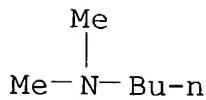
RN 927-62-8 HCA

CN 1-Butanamine, N,N-dimethyl- (9CI) (CA INDEX NAME)



IC ICM C12Q
 CC 3-1 (Biochemical Genetics)
 IT 64-18-6, Formic acid, uses 64-19-7, Acetic acid, uses 67-56-1,
 Methanol, uses 75-05-8, Acetonitrile, uses 79-09-4, Propionic
 acid, uses 98-94-2, N,N-Dimethylcyclohexylamine 108-18-9,
 Diisopropylamine 121-44-8, Triethylamine, uses 124-02-7,
 Diallylamine 463-79-6, Carbonic acid, uses 927-62-8,
 N,N-Dimethylbutylamine 996-35-0, N,N-Dimethylisopropylamine
 1185-53-1, Tris hydrochloride 7447-40-7, Potassium chloride, uses
 7487-88-9, Magnesium sulfate, uses 7783-20-2, Ammonium sulfate,
 uses
 (sequencing kit contg.; nucleic acid sequencing using nicking
 agents and linear or exponential amplification under isothermal
 conditions)

L40 ANSWER 2 OF 12 HCA COPYRIGHT 2004 ACS on STN
 138:187378 Enhanced product selectivity in continuous N-methylation of
 amino alcohols over solid acid-base catalysts with supercritical
 methanol. Oku, Tomoharu; Ikariya, Takao (Graduate School of Science
 and Engineering, Tokyo Institute of Technology, Tokyo, 152-8552,
 Japan). Angewandte Chemie, International Edition, 41(18), 3476-3479
 (English) 2002. CODEN: ACIEF5. ISSN: 1433-7851. OTHER SOURCES:
 CASREACT 138:187378. Publisher: Wiley-VCH Verlag GmbH & Co. KGaA.
 AB The unique properties of supercrit. fluids can be exploited for
 fine-tuning product selectivity. Under the conditions listed for
 the N-methylation of amino alcs. over solid acid-base bifunctional
 catalysts, the total yield and product selectivity could be
 improved. Enhanced product selectivity might be attributed to the
 milder reaction conditions possible with supercrit. methanol, as
 well as the increased concn. of methanol on the catalyst.
 IT 927-62-8P, 1-Butanamine, n,n-dimethyl-
 (effect of water on continuous N-methylation of amino alcs. with
 supercrit. methanol in presence of solid acid-base catalysts)
 RN 927-62-8 HCA
 CN 1-Butanamine, N,N-dimethyl- (9CI) (CA INDEX NAME)



CC 23-7 (Aliphatic Compounds)

IT H-Beta **zeolites**

Hydrogen **mordenite-type zeolites**

Oxides (inorganic), uses

(continuous N-methylation of amino alcs. with supercrit. methanol in presence of solid acid-base catalysts)

IT 100-61-8P, Aniline, n-methyl-, preparation 110-68-9P,
 1-Butanamine, n-methyl- 121-69-7P, Aniline, n,n-dimethyl-,
 preparation 872-50-4P, 2-Pyrrolidinone, 1-methyl-, preparation
927-62-8P, 1-Butanamine, n,n-dimethyl- 1704-62-7P,
 Ethanol, 2-[2-(dimethylamino)ethoxy]- 2751-70-4P, 1-Pentanol,
 5-(methylamino)- 2893-43-8P, Ethanol, 2-(ethylmethylamino)-
 2893-49-4P, Ethanol, 2-[methyl-(1-methylethyl)amino]- 3179-63-3P,
 1-Propanol, 3-(dimethylamino)- 13330-96-6P, 1-Butanol,
 4-(dimethylamino)- 26311-17-1P, Ethanamine, 2-ethoxy-n,N-dimethyl-
 27384-58-3P, 1-Pentanol, 5-(dimethylamino)- 38256-94-9P,
 Ethanamine, 2-ethoxy-n-methyl- 42042-68-2P, 1-Butanol,
 4-(methylamino)- 42055-15-2P, 1-Propanol, 3-(methylamino)-
 85475-01-0P, Ethanol, 2-[2-(methylamino)ethoxy]-
 (effect of water on continuous N-methylation of amino alcs. with
 supercrit. methanol in presence of solid acid-base catalysts)

L40 ANSWER 3 OF 12 HCA COPYRIGHT 2004 ACS on STN

136:306404 Genotyping by liquid chromatographic analysis of short nucleic acid fragments. Van Ness, Jeffrey; Galas, David J.; Garrison, Lori K. (Keck Graduate Institute, USA). PCT Int. Appl. WO 2002028501 A1 20020411, 74 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2001-US30828 20011001. PRIORITY: US 2000-PV237409 20001002; US 2000-PV247173 20001110; US 2000-PV247172 20001110; US 2000-PV247275 20001110; US 2000-PV247166 20001110; US 2000-PV247167 20001110; US 2001-PV263971 20010124; US 2001-PV269244 20010215; US 2001-PV300319 20010621; US 2001-PV300350 20010621; US 2001-PV301394 20010627.

AB The invention concerns genotyping anal. by liq. chromatog. anal. of short nucleic acid fragments. The nucleic acid fragments are

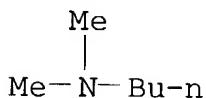
amplification products using specifically designed oligonucleotides as primers and target nucleic acids contg. nucleotides of interest as **templates**. The oligonucleotides contain recognition sequences for restriction endonucleases that cleave outside the recognition sequences. The short nucleic acid fragments can be rapidly and reliably analyzed using liq. chromatog., optionally followed by mass spectrometry, and the nucleotides of interest identified.

IT 927-62-8

(genotyping by liq. chromatog. anal. of short nucleic acid fragments)

RN 927-62-8 HCA

CN 1-Butanamine, N,N-dimethyl- (9CI) (CA INDEX NAME)



IC ICM B01D015-08

CC 9-3 (Biochemical Methods)

Section cross-reference(s): 3

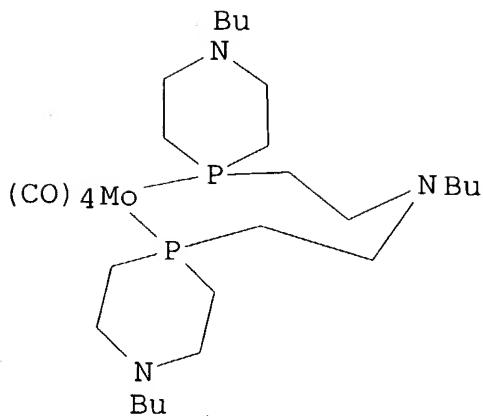
IT 64-18-6, Formic acid, uses 64-19-7, Acetic acid, uses 64-19-7D, Acetic acid, halogenated derivs. 67-56-1, Methanol, uses 71-52-3, Bicarbonate, uses 75-05-8, Acetonitrile, uses 79-09-4, Propionic acid, uses 79-09-4D, Propionic acid, halogenated derivs. 98-94-2, N,N-Dimethylcyclohexylamine 108-18-9, Diisopropylamine 121-44-8, Triethylamine, uses 124-02-7, Diallylamine 927-62-8 996-35-0, N,N-Dimethylisopropylamine . 3812-32-6, Carbonate, uses 7647-01-0, Hydrochloric acid, uses 9012-90-2, DNA Polymerase

(genotyping by liq. chromatog. anal. of short nucleic acid fragments)

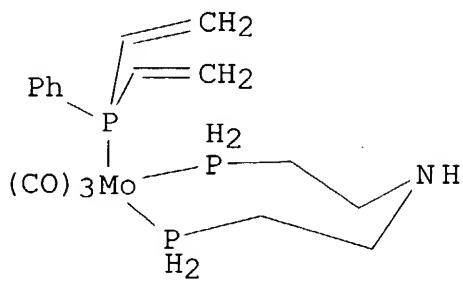
L40 ANSWER 4 OF 12 HCA COPYRIGHT 2004 ACS on STN

129:16172 Water-soluble phosphines. VII. Synthesis, coordination chemistry and **template** reactions of pH-functional bis(phosphinoethyl)amines. Hessler, Antonella; Kucken, Stefan; Stelzer, Othmar; Sheldrick, William S. (Anorganische Chemie, Fachbereich 9, Bergische Universitat-GH Wuppertal, Wuppertal, D-42097, Germany). Journal of Organometallic Chemistry, 553(1-2), 39-52 (German) 1998. CODEN: JORCAI. ISSN: 0022-328X. Publisher: Elsevier Science S.A..

GI



I



II

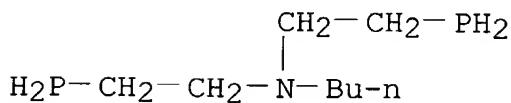
AB Diprimary and disecondary bis(phosphinoethyl)amines $\text{RN}[(\text{CH}_2)_2\text{PHR}']_2$ ($\text{R} = \text{H, Bu, p-Tol}$; $\text{R}' = \text{H, Ph}$) (1a-1c, 2a) in addn. to azaphosphorinanes are accessible by alkylation of PH_3 or primary phosphines with bis(chloroethyl)amines in the superbasic medium DMSO/KOH . Sequential P-methylation and N,P-silylation of 1a yields $\text{HN}[(\text{CH}_2)_2\text{PHMe}]_2$ (2b) and the N- and P-trimethylsilyl derivs. $\text{Me}_3\text{SiN}[(\text{CH}_2)_2\text{PHMe}]_2$ (3a) and $\text{Me}_3\text{SiN}[(\text{CH}_2)_2\text{P}(\text{SiMe}_3)\text{Me}]_2$ (3c). With $\text{C}_7\text{H}_8\text{Mo}(\text{CO})_3$ the potentially tridentate P2N hybrid ligands 1a, 1b (L) form kinetically labile complexes fac- $\text{Mo}(\text{CO})_3(\text{L})$ (4a, 4b). Eight membered chelate complexes cis- $\text{Mo}(\text{CO})_4(\text{L})$ (4c, 5a) are obtained on reaction of 1b and 2b (L) with $\text{C}_7\text{H}_8\text{Mo}(\text{CO})_4$, the ligands L acting as P,P-bidentates. The x-ray structure of 4c (space group Pbca) reveals a distorted eight membered chelate ring system. By periphery reactions (P-metalation, N-protonation and complexation with borane) a series of derivs. are accessible. A complex of a bidentate ligand with terminal azaphosphorinane units I is obtained by alkylation with $\text{nBuN}[(\text{CH}_2)_2\text{Cl}]_2$. Attempts to form a twelve membered tetradentate macrocycle by template mediated PH/C:C addn. of divinylphenylphosphine to 4a, 4b failed, however. The x-ray structure of the template II (space group $\text{P}21/c$) formed initially from 4a shows the $\text{PhP}(\text{CH}=\text{CH}_2)_2$ ligand to be in cis-position to the diprimary phosphine which is coordinated to molybdenum via its P-atoms forming a folded eight membered ring system.

IT 207689-13-2P

(synthesis, coordination chem., and template reactions of phosphorus-hydrogen functional bis(phosphinoethyl)amines)

RN 207689-13-2 HCA

CN 1-Butanamine, N,N-bis(2-phosphinoethyl)- (9CI) (CA INDEX NAME)



CC 29-7 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 75, 78

ST **template** phosphinoethyl amine prepn reaction; crystal structure phosphinoethyl amine molybdenum complex; mol structure phosphinoethyl amine molybdenum complex

IT 207689-23-4P

(crystal structure; synthesis, coordination chem., and **template** reactions of phosphorus-hydrogen functional bis(phosphinoethyl)amines)

IT 638-21-1, Phenylphosphine 821-48-7 6399-81-1, Triphenylphosphine hydrobromide 7803-51-2, Phosphine 12125-77-8 12146-37-1 26681-88-9, Divinylphenylphosphine 55112-89-5 102837-01-4 (synthesis, coordination chem., and **template** reactions of phosphorus-hydrogen functional bis(phosphinoethyl)amines)

IT 170471-27-9P 207689-12-1P **207689-13-2P** 207689-14-3P 207689-17-6P 207689-19-8P 207689-21-2P 207689-22-3P 207689-24-5P 207689-25-6P 207689-29-0P (synthesis, coordination chem., and **template** reactions of phosphorus-hydrogen functional bis(phosphinoethyl)amines)

L40 ANSWER 5 OF 12 HCA COPYRIGHT 2004 ACS on STN

124:109289 Clinical pathology changes related to cutaneous irritation in the Fischer 344 rat and New Zealand White rabbit. Hermansky, Steven J.; Neptun, Douglas A.; Weaver, Elizabeth V.; Ballantyne, Bryan (North American Science Associates, Northwood, OH, 43619-1397, USA). Journal of Toxicology, Cutaneous and Ocular Toxicology, 14(4), 219-36 (English) 1995. CODEN: JTOTDO. ISSN: 0731-3829. Publisher: Dekker.

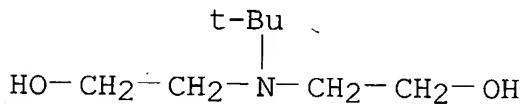
AB An evaluation of 27 repeated dose cutaneous application studies (9 applications of 6 h over an 11-day period) indicated that several hematol. and clin. chem. parameters may be altered by chem. induced skin irritation. Irresp. of species, values that were generally decreased included Hb concn., hematocrit, erythrocyte count, and serum concns. of calcium, potassium, inorg. phosphorus, and creatinine. Values that were increased included the neutrophil and total leukocyte counts. Some species differences were seen; for example, while the **platelet** count and serum globulin concn. were increased in rabbits only, the serum glucose, sodium, and chloride concns. were increased in rats only. The mean corpuscular vol. (MCV), mean corpuscular Hb (MCH), and serum albumin and total protein concns. were variably affected. Changes were

generally well assocd. with the degree of cutaneous irritation, but did not appear to be related to the chem. class of the test substances, decreased food consumption, loss of body wt., or systemic toxicity of the chem.

IT 2160-93-2, tert-Butyldiethanolamine
(chem. toxicity and cutaneous irritation in relation to changes in clin. pathol.)

RN 2160-93-2 HCA

CN Ethanol, 2,2'-(1,1-dimethylethyl)imino]bis- (9CI) (CA INDEX NAME)



CC 4-3 (Toxicology)

IT Blood platelet
Erythrocyte
Hematocrit
Leukocyte
(chem. toxicity and cutaneous irritation in relation to changes in clin. pathol.)

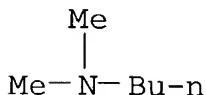
IT 108-01-0, n,n-Dimethylethanamine 111-42-2, biological studies
112-25-4, Ethylene glycol monohexyl ether 112-59-4 1704-62-7,
2-(2-Dimethylamino)ethoxy)ethanol 1760-24-3 2160-93-2,
tert-Butyldiethanolamine 9012-76-4D, Chitosan, pyrrolidone
carboxylic acid salts 9016-00-6D, PolyDimethylsiloxane, derivs.
9036-19-5, Octylphenoxypropoxyethanol 9063-89-2,
Polyoxyethylene octyl phenyl ether 16881-77-9,
Methyldimethoxysilane 17268-47-2, 3-Dimethylamino-n,n-dimethylpropionamide 18268-70-7, Tetraethylene glycol di(2-ethyl hexoate) 24991-55-7, Polyethylene glycol dimethyl ether 25322-68-3D, derivs. 31900-57-9D, PolyDimethylsiloxane, derivs.
34911-46-1 38433-80-6 101003-79-6 148411-57-8 173106-98-4D,
ethoxylated gluco derivs.
(chem. toxicity and cutaneous irritation in relation to changes in clin. pathol.)

L40 ANSWER 6 OF 12 HCA COPYRIGHT 2004 ACS on STN
123:286870 In situ preparation of N,N-dimethyl-n-butylamine for 2,6-dimethylphenol polymerization. Li, Kuo-Tseng; Lin, Chen-Chin (Dep. Chem. Eng., Tunghai Univ., Taichung, Taiwan). Journal of Applied Polymer Science, 58(7), 1199-204 (English) 1995. CODEN: JAPNAB. ISSN: 0021-8995. Publisher: Wiley.

AB 2,6-Dimethylphenol (2,6-DMP) polymn. with a catalytic complex of Cu2O/HBr/N,N'-di-tert-butylethylenediamine/BuNMe2/Bu2NH was studied, in which BuNMe2 was prep'd. in situ from MeOH and BuNH2 over 4 different solid acid catalysts (2 γ -alumina, 1 silica-alumina,

1 **zeolite**). The effectiveness of the unpurified methylation product solns. for promoting 2,6-DMP polymn. depended strongly on the type of solid acid catalyst, with the performance of the best (an alumina) being very similar to that of reagent-grade BuNMe₂. IR spectral studies showed that BuNMe₂ acted as the external base for the polymn. catalyst system to neutralize the excess HBr and to increase the polymn. rate.

IT **927-62-8P**, Butyldimethylamine
(catalyst component; in-situ prepn. of dimethylbutylamine for dimethylphenol polymn.)
RN 927-62-8 HCA
CN 1-Butanamine, N,N-dimethyl- (9CI) (CA INDEX NAME)

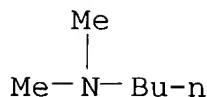


CC 35-3 (Chemistry of Synthetic High Polymers)
IT **Zeolites**, uses
(rare earth Y, methylation catalysts; in-situ prepn. of dimethylbutylamine for dimethylphenol polymn.)
IT **927-62-8P**, Butyldimethylamine
(catalyst component; in-situ prepn. of dimethylbutylamine for dimethylphenol polymn.)

L40 ANSWER 7 OF 12 HCA COPYRIGHT 2004 ACS on STN
120:220770 Methylation of n-butylamine over solid-acid catalysts. Li, Kuo-Tseng; Peng, Yuan-Chu (Department of Chemical Engineering, Tunghai University, Taichung, Taiwan). Applied Catalysis, A: General, 109(2), 225-33 (English) 1994. CODEN: ACAGE4. ISSN: 0926-860X.

AB N,N-dimethyl-n-butylamine was synthesized with a good yield by the reaction between BuNH₂ and MeOH over a variety of solid-acid catalysts. Activity measurements were carried out with a flow reactor at 220-340°. The measured catalytic activity decreased in the order: rare-earth ion-exchanged **zeolite** Y.apprxeq.**zeolite** beta>TiO₂-ZrO₂>**zeolite** NaY.apprxeq.**zeolite** mordenite>low-Na γ -alumina> **zeolite** X>silica-alumina>high-Na γ -alumina> **zeolite** L>**zeolite** 5A. Comparisons between the activity measurements and temp.-programmed desorption studies suggested that the BuNH₂ methylation rate was highly dependent on the strength of acid sites.

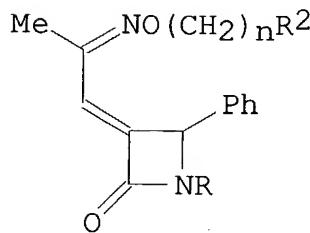
IT **927-62-8P**, N,N-Dimethyl-n-butylamine
(prepn. of, by methylation of butylamine over acid catalysts)
RN 927-62-8 HCA
CN 1-Butanamine, N,N-dimethyl- (9CI) (CA INDEX NAME)



CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
 Section cross-reference(s): 23
 IT **Zeolites**, uses
 (5A, catalysts, for methylation of butylamine with methanol)
 IT **Zeolites**, uses
 (L, catalysts, for methylation of butylamine with methanol)
 IT **Zeolites**, uses
 (NaY, catalysts, for methylation of butylamine with methanol)
 IT **Zeolites**, uses
 (X, catalysts, for methylation of butylamine with methanol)
 IT **Zeolites**, uses
 (Y, catalysts, for methylation of butylamine with methanol)
 IT **Zeolites**, uses
 (beta, catalysts, for methylation of butylamine with methanol)
 IT 1314-23-4, Zirconia, uses 12173-98-7, **Mordenite**
 13463-67-7, Titania, uses
 (catalysts, for methylation of butylamine with methanol)
 IT **927-62-8P**, N,N-Dimethyl-n-butylamine
 (prepn. of, by methylation of butylamine over acid catalysts)

L40 ANSWER 8 OF 12 HCA COPYRIGHT 2004 ACS on STN
 113:171863 Preparation of 3-[(aminoalkoxy)imino]propylidene]azetidinone
 s as **platelet aggregation inhibitors**. Kawashima, Yutaka;
 Sato, Masakazu; Kawase, Masahiro; Watanabe, Yoshiaki; Hatayama,
 Katsuo (Taisho Pharmaceutical Co., Ltd., Japan). Eur. Pat. Appl. EP
 365364 A2 19900425, 10 pp. DESIGNATED STATES: R: AT, BE, CH, DE,
 FR, GB, IT, LI, LU, NL, SE. (English). CODEN: EPXXDW.
 APPLICATION: EP 1989-310857 19891020. PRIORITY: JP 1988-265183
 19881020.

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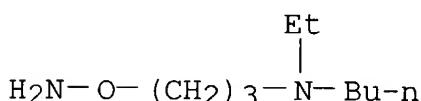
AB The title compds. [I; R = halophenyl, alkylphenyl, alkoxy(carbonyl)phenyl; R2 = NR3R4, (un)substituted piperidino, piperazino, **morpholino**, etc.; R3, R4 = H, alkenyl, Ph, PhCH2; n = 2-10] were prepd. Thus, (E)-1-(4-methoxyphenyl)-3-(2-oxopropylidene)-4-phenyl-2-azetidinone was stirred overnight with HONH2.HCl in Me2CHOH and the product stirred, in turn, with NaH and then with 1-(3-chloropropyl)-4-(2-pyridyl)piperidine in DMF to give I [R = 4-(MeO)C6H4, R2 = 4-(2-pyridyl)piperidino, n = 3] which gave 57.61% inhibition of ADP-induced thrombocytopenia in mice at 300 mg/kg orally.

IT **127437-53-0P**

(prepn. and reaction of, in prepn. of **platelet aggregation inhibitors**)

RN 127437-53-0 HCA

CN 1-Butanamine, N-[3-(aminoxy)propyl]-N-ethyl- (9CI) (CA INDEX NAME)



IC ICM C07D205-08

ICS C07D401-12; A61K031-395

CC 27-5 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 1

ST aminoalkoxyiminopropylideneazetidinone prepn **platelet inhibitor**; azetidinone aminoalkoxyiminopropylidene prepn **platelet inhibitor**

IT Blood **platelet aggregation inhibitors**

([(aminoalkoxy)imino]propylidene]azetidinones)

IT 127437-45-0P 127437-46-1P 127437-49-4P **127437-53-0P**

129722-76-5P 129722-77-6P

(prepn. and reaction of, in prepn. of **platelet aggregation inhibitors**)

IT	129722-35-6P	129722-36-7P	129722-38-9P	129722-39-0P
	129722-40-3P	129722-42-5P	129722-43-6P	129722-44-7P
	129722-45-8P	129722-46-9P	129722-47-0P	129722-49-2P
	129722-50-5P	129722-51-6P	129722-52-7P	129722-53-8P
	129722-54-9P	129722-55-0P	129722-56-1P	129722-57-2P
	129722-58-3P	129722-59-4P	129722-60-7P	129722-61-8P
	129722-62-9P	129722-63-0P	129722-64-1P	129722-65-2P
	129722-66-3P	129722-67-4P	129722-68-5P	129722-69-6P
	129722-70-9P	129722-71-0P	129722-72-1P	129722-73-2P
	129722-74-3P	129722-75-4P	129722-82-3P	129741-40-8P
	129889-45-8P			

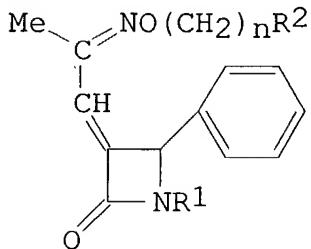
(prepn. of, as **platelet aggregation inhibitor**)

IT 524-38-9 36421-15-5, 3-Chloropropylbutilamine 115738-05-1
116254-32-1 127437-48-3 129722-78-7

(reaction of, in prepn. of **platelet** aggregation inhibitors)

L40 ANSWER 9 OF 12 HCA COPYRIGHT 2004 ACS on STN
 113:115062 Preparaton of 1-benzyl-3-[2-(diaminoalkoxyimino)propylidene]-4-phenyl-2-azetidinones as blood **platelet** aggregation inhibitors. Kawashima, Yutaka; Sato, Masakazu; Hatada, Yuichi; Nakajima, Yoshimoto; Soda, Kaoru (Taisho Pharmaceutical Co., Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 01246256 A2 19891002 Heisei, 7 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1988-72667 19880326.

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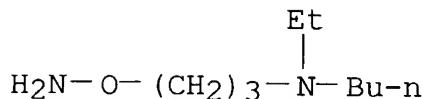
I

AB The title compds. I [R¹ = (halo)benzyl; R² = NR³R⁴, pyrrolidyl, (lower alkyl or benzyl)piperidyl, tetrahydroazepinyl, (lower alkyl) **morpholinyl**; R³, R⁴ = alkyl, lower alkenyl; n = 1-3] are prep'd. MeCOCH₂:PPh₃ (2.98 g) was treated with 2.35 g 1-benzyl-4-phenyl-2,3-azetidinedione in C₆H₆ at room temp. overnight to give 2.18 g (E)-1-benzyl-3-(2-oxopropylidene)-4-phenyl-2-azetidinone (II). A DMF suspension of NaH was stirred with 11.9 g N-hydroxyphthalimide in DMF for 30 min and the reaction mixt. was treated with 15 g Bu₂N(CH₂)₃Cl in DMF under reflux for 5 h to give 23.4 g N-(3-dibutylaminopropoxy)phthalimide, which in CH₂Cl₂ was treated with 20 mL H₂NNH₂.H₂O at room temp. for 3 h to give 10.3 g Bu₂N(CH₂)₃ONH₂ (III). A mixt. of II 1.5 g, III 1.04 g, and 10-camphorsulfonic acid 50 mg in C₆H₆ was refluxed for 3 h and the resulting product was treated with AcOEt soln. of HCl to give 1.0 g (E)-I.HCl (R¹ = CH₂Ph, R² = NBu₂, n = 3), whose inhibition rate against blood **platelet** aggregation (ex vivo in rat) was 121%, vs. 100% for ticlopidine.

IT 127437-53-0P, O-[3-(Butylethylamino)propyl]hydroxylamine (prep. and condensation of, with (oxopropylidene)azetidinone, (aminopropoxyimino)propylideneazetidinone from)

RN 127437-53-0 HCA

CN 1-Butanamine, N-[3-(aminoxy)propyl]-N-ethyl- (9CI) (CA INDEX NAME)



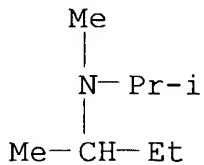
IC ICM C07D205-10
 ICS A61K031-395; A61K031-445; A61K031-55; C07D401-12; C07D403-12;
 C07D409-12
 CC 27-5 (Heterocyclic Compounds (One Hetero Atom))
 Section cross-reference(s): 1
 ST azetidinone aminoalkoxyiminopropylidene **platelet**
 aggregation inhibitor; aminoalkoxyiminopropylideneazetidinone prepn
platelet aggregation inhibitor; phenylbenzylazetidinone
 aminoalkoxyiminopropylidene **platelet** aggregation
 inhibitor; benzylphenylazetidinone aminoalkoxyiminopropylidene
platelet aggregation inhibitor
 IT Blood **platelet** aggregation inhibitors
 (benzyl[(aminoalkoxyimino)propylidene]phenylazetidinones)
 IT 127303-75-7P 127437-46-1P, O-(3-Dibutylaminopropyl)hydroxylamine
 127437-47-2P, O-(3-Pyrrolidylpropyl)hydroxylamine 127437-48-3P,
 O-(Piperidylpropyl)hydroxylamine 127437-49-4P 127437-50-7P
 127437-51-8P 127437-52-9P, O-[3-(Diethylamino)propyl]hydroxylamine
127437-53-0P, O-[3-(Butylethylamino)propyl]hydroxylamine
 127437-54-1P 127437-55-2P, O-[3-(Diallylamino)propyl]hydroxylamine
 127437-56-3P 127437-57-4P
 (prepn. and condensation of, with (oxopropylidene)azetidinone,
 (aminopropoxyimino)propylideneazetidinone from)
 IT 127303-77-9P 127437-58-5P 127437-59-6P 127437-60-9P
 127437-61-0P 127437-62-1P 127437-63-2P 127437-64-3P
 127437-65-4P 127437-66-5P 127437-67-6P 127437-68-7P
 127437-69-8P 127437-70-1P 127437-71-2P 127437-72-3P
 127437-73-4P 127437-74-5P
 (prepn. of, as blood **platelet** aggregation inhibitor)

L40 ANSWER 10 OF 12 HCA COPYRIGHT 2004 ACS on STN
 93:25895 Tertiary amines by reductive alkylation. Decker, Quintin W.;
 Marcus, Erich (Union Carbide Corp., USA). U.S. US 4190601 19800226,
 7 pp. (English). CODEN: USXXAM. APPLICATION: US 1978-911096
 19780531.

AB RCH₂NHCH₂R₁ (R and R₁ are alkyl, cycloalkyl, hydroxyalkyl, aralkyl,
 H) were treated with aliph. aldehydes and ketones and H over
 hydrogenation catalysts at 20-200° to give the resp.
 RCH₂N(CH₂R₁)CHR₂R₃ (R₂ and R₃ are each alkyl or H, or CR₂R₃ is a
 cycloalkylidene group). The reaction of [HO(CH₂)₃]₂NH with Me₂CO
 and H over Ni and a **zeolite** gave [HO(CH₂)₃]₂NCHMe₂.

IT 74012-02-5P
 (prepn. of)
 RN 74012-02-5 HCA

CN 2-Butanamine, N-methyl-N-(1-methylethyl)- (9CI) (CA INDEX NAME)



IC C07C085-08

NCL 260583000R

CC 23-4 (Aliphatic Compounds)

IT 34753-59-8P 74012-02-5P

(prep. of)

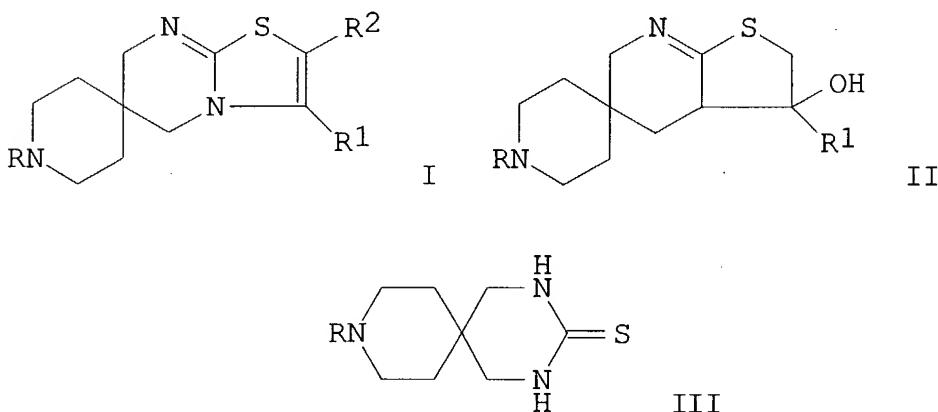
L40 ANSWER 11 OF 12 HCA COPYRIGHT 2004 ACS on STN

85:177356 Spiro[piperidine-4,6'-thiazolo[3,2-a]pyrimidines].

Thymoanaleptics and blood platelet aggregation inhibitors.

Szarvasi, Etienne; Festal, Didier; Grand, Marcel; Depin, Jean C.; Chabert, Janine (Soc. LIPHA, Lyons, Fr.). European Journal of Medicinal Chemistry, 11(2), 115-24 (French) 1976. CODEN: EJMCA5. ISSN: 0323-5234

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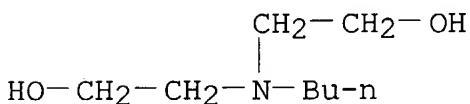
AB Spiropiperidinethiazolopyrimidines I ($R = Bu, octyl, CH_2Ph; R_1 = Ph, 4-FC_6H_4, 2-MeOC_6H_4, 2-naphthyl, 2,5-(MeO)2CH_3, 2-furyl, 2-thienyl, 3,4-C_12C_6H_3, R_2 = H; R = Bu, R_1 = Ph, R_2 = Me, Ph$) and II ($R = Bu, octyl, decyl, cyclohexyl, CH_2Ph, 1-naphthylmethyl, 3,4-(MeO)2C_6H_3CH_2, 3,4-C_12C_6H_3CH_2; R_1 = Ph, 2-naphthyl, 2,5-(MeO)2C_6H_3, 2-MeOC_6H_4, 3,4-C_12C_6H_3, 4-PhC_6H_4, 4-O_2NC_6H_4$) were

prepd. by treating thiones III with R₁COCHR₂Br. III were obtained from diethanolamine in 5 steps. II (R = arom., R₁ = 3,4-C₁₂C₆H₃, R₂ = H) are antidepressants, and I (R = aliph., 2,5-(MeO)C₆H₃) are platelet aggregation inhibitors.

IT 102-79-4P
(prepn. and chlorination of)

RN 102-79-4 HCA

CN Ethanol, 2,2'-(butylimino)bis- (9CI) (CA INDEX NAME)



CC 28-17 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

IT Blood platelet
(aggregation of, inhibition of, by spiropiperidinethiazolopyrimidines)

IT 101-32-6P 102-79-4P 1541-67-9P 4500-29-2P
15520-05-5P 19344-33-3P 20109-33-5P 60855-80-3P 60855-81-4P
60876-94-0P

(prepn. and chlorination of)

IT 52419-67-7P 52419-70-2P 52419-76-8P 52419-77-9P 52488-15-0P
52501-97-0P 60856-20-4P 60856-45-3P

(prepn. and platelet aggregation-inhibiting activity of)

IT 52419-69-9P 52419-72-4P 52761-37-2P
(prepn. and platelet aggregation-inhibiting and antidepressant activity of)

L40 ANSWER 12 OF 12 HCA COPYRIGHT 2004 ACS on STN

54:2316 Original Reference No. 54:570h-i,571a-i,572a-e

3-Tetrahydrofuryl-substituted ammonium compounds. Eugster, Conrad H.; Denss, Rolf; Hafliger, Franz; Hofer, Bruno; Pfister, Rudolf; Zimmermann, Markus (Geigy Chemical Corp.). US 2895965 19590721 (Unavailable). APPLICATION: US .

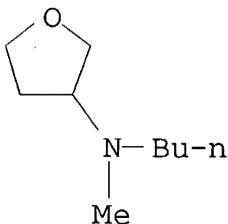
AB The title compds. had strong neurophysiol. activity, being in particular strong vasodilators, useful in the treatment of hypertension and other circulatory diseases. Thus, 3-dimethylamino-5-ethyltetrahydrofuran (I), b₁₁ 60-2°, (1 g.) treated with 1 cc. MeI gave I.MeI (Ia), m. 140.5-1° (EtOH-Et₂O). Ia treated with AgCl gave I.MeCl, m. 150-1° (EtOH-Et₂O), very hygroscopic. Also prep'd. were: I.AuCl₄, m. 116-17° (water), as yellow platelets; from 3-dimethylaminotetrahydrofuran (II), b₈₀ 77-8°, the HCl salt, m. 138-40°, the MeI salt (IIa), m. 226-6.5° (EtOH-Et₂O); II MeCl salt (IIb), m. 298-9° (iso-PrOH-acetone),

benzyloxyhexane (XXIX), b0.001 132°. XXIX was treated with 66% H₂SO₄ to give dl-XX. XXVI treated with Me₃N gave XX methobromide, oil. CH₂:CHCH₂MgBr was treated with benzyloxyacetaldehyde to give benzyloxymethylallylcarbinol (XXX), b0.006 82-5°. XXX treated with Br followed by pulverized KOH gave 3-bromo-5-benzyloxymethyltetrahydrofuran (XXXI), b0.005 111-18°. XXXI treated with Me₂NH gave 3-dimethylamino-5-benzyloxymethyltetrahydrofuran (XXXII), b0.004 98-9°. 1,4-Dihydroxy-2-dimethylamino-5-benzyloxypentane (XXXIII) in pyridine was treated with MeSO₂Cl to give XXXII. XXXII was reduced over Pd-C with H to give 3-dimethylamino-5-hydroxymethyltetrahydrofuran (XXXIV), b11 112-20°. XXXIV with Ac₂O gave the HOAc ester, b0.003 62-4°. XXXIV yielded a perchlorate, m. 78-81° (MeOH-EtOAc). XXXIII with H₂SO₄ gave XXXIV. Benzyl glycide ether was converted to α -acetyl- δ -benzyloxy- γ -valerolactone, b0.001 152°, then α -oxo- δ -benzyloxy- γ -valerolactone phenylhydrazone, m. 169°, which gave α -formylamino- δ -benzyloxy- γ -valerolactone and finally XXXIII from α -dimethylamino- δ -benzyloxy- γ -valerolactone, b0.05 155°. XXXIV treated with MeI gave XXXIV methiodide which did not crystallize. Treatment with Ac₂O gave N-(5-acetoxyethyl-3-tetrahydrofuryl)-N,N,N-trimethylammonium iodide, m. 177-80°.

IT 91425-91-1, 3-Furanamine, N-butyltetrahydro-N-methyl-
(prepn. of)

RN 91425-91-1 HCA

CN 3-Furanamine, N-butyltetrahydro-N-methyl- (6CI, 7CI) (CA INDEX
NAME)



CC 10G (Organic Chemistry: Heterocyclic Compounds)

IT 2,5-Hexanediol, 3-dimethylamino-, dl-

Ammonium, (2,5-diethyltetrahydro-2,5-dimethyl-3-furyl)trimethyl-, iodide

Ammonium, (2-ethyltetrahydro-3-furyl)trimethyl-, iodide

Ammonium, [3-hydroxy-1-(1-hydroxyethyl)butyl]trimethyl-, iodide

Ammonium, [5-(2-bromovinyl)tetrahydro-3-furyl]trimethyl-, iodide

Ammonium, allyldimethyl(tetrahydro-5-methyl-3-furyl)-, bromide

Ammonium, benzyldimethyl(tetrahydro-3-furyl)-, iodide

Ammonium, butyldimethyl(tetrahydro-3-furyl)-, iodide

Ammonium, diethylmethyl(tetrahydro-3-furyl)-, iodide
 Ammonium, trimethyl(tetrahydro-2,5-dimethyl-3-furyl)-, iodide
 Ammonium, trimethyl(tetrahydro-5-methyl-3-furyl)-, iodide
 Ammonium, trimethyl(tetrahydro-5-phenyl-3-furyl)-, iodide
 Ammonium, trimethyl[tetrahydro-5-(hydroxymethyl)-3-furyl]-, acetate
 Ammonium, trimethyl[tetrahydro-5-(hydroxymethyl)-3-furyl]-, iodide
 Furfuryl alcohol, 4-bromotetrahydro- α -methyl-, dl-

Morpholinium compounds, 4-methyl-4-tetrahydro-3-furyl-, iodide

IT Piperidinium, 1-methyl-1-tetrahydro-3-furyl-, iodide
 13606-79-6, Morpholine, 4-tetrahydro-3-furyl-
 58931-16-1, 4-Penten-2-ol, 1-(benzyloxy)- 89854-99-9,
 3-Furanamine, tetrahydro-N,N,5-trimethyl- 90226-64-5,
 3-Furanamine, 2-ethyltetrahydro-N,N-dimethyl- 90226-66-7,
 3-Furanamine, tetrahydro-N,N,2,5-tetramethyl- 90949-67-0,
 Piperidine, 1-tetrahydro-3-furyl- 91425-91-1,
 3-Furanamine, N-butyltetrahydro-N-methyl- 92920-38-2, Valeric acid, 2-acetyl-5-(benzyloxy)-4-hydroxy-, γ -lactone
 93137-49-6, 3-Furanamine, 2,5-diethyltetrahydro-N,N,2,5-tetramethyl-
 98022-86-7, 1-Butanesulfonic acid, 3,4-dibromo-1-hydroxy-
 98491-97-5, 3-Furanamine, 5-(2-bromovinyl)tetrahydro-N,N-dimethyl-
 99595-90-1, 3-Furoic acid, 5-acetyl-, methyl ester 99968-61-3,
 Ketone, 5-bromotetrahydro-2-furyl methyl 100058-60-4, Butane, 3-(benzyloxy)-1,2-epoxy- 100368-85-2, 3-Furanamine, N-butyltetrahydro-N-methyl- 100368-86-3, 3-Furanamine, tetrahydro-N,N-dimethyl-5-phenyl- 100388-05-4, Furan, 2-[(benzyloxy)methyl]-4-bromotetrahydro- 100967-30-4,
 1,4-Pantanediol, 5-(benzyloxy)-2-dimethylamino- 101086-57-1,
 1,4-Hexanediol, 5-(benzyloxy)-2-dimethylamino- 101257-76-5,
 3-Furanamine, N,N-diethyltetrahydro- 101776-05-0, 3-Furanamine, 5-[(benzyloxy)methyl]tetrahydro-N,N-dimethyl- 101793-70-8, Valeric acid, 5-(benzyloxy)-4-hydroxy-2-oxo-, γ -lactone, phenylhydrazone 102005-61-8, Hexanoic acid, 5-(benzyloxy)-2-dimethylamino-4-hydroxy-, γ -lactone 102081-49-2, Hexanoic acid, 5-(benzyloxy)-4-hydroxy-2-oxo-, γ -lactone, phenylhydrazone 105338-71-4, Ketone, 5-bromotetrahydro-2-furyl methyl, (2,4-dinitrophenyl)hydrazone 106740-55-0, Hexanoic acid, 2-acetyl-5-(benzyloxy)-4-hydroxy-, γ -lactone 109535-11-7, Norleucine, 5-(benzyloxy)-N-formyl-4-hydroxy-, γ -lactone 109535-12-8, Norvaline, 5-(benzyloxy)-N-formyl-4-hydroxy-, γ -lactone 109650-47-7, Norvaline, 5-(benzyloxy)-4-hydroxy-N,N-dimethyl-, γ -lactone 112485-00-4, 2-Furonitrile, 5-bromotetrahydro- (prepn. of).